NATIONAL BUREAU OF STANDARDS REPORT

9968

FIFTEENTH REPORT ON
A SURVEY OF THERMODYNAMIC PROPERTIES OF THE COMPOUNDS OF THE ELEMENTS CHNOPS

Progress Report for the Period 1 July to 31 December 1968

to

National Aeronautics and Space Administration

20 December 1968

NBS

U.S. DEPARTMENT OF COMMERCE

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George T. Armstrong and Eugene S. Domalski

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Contract No. R-138, Amendment 3

U.S. DEPARTMENT OF COMMERCE

NATIONAL BUREAU OF STANDARDS

FOREWORD

A Study at the National Bureau of Standards (NBS), of which this is the fifteenth progress report, has been undertaken to meet the need of the National Aeronautics and Space Administration (NASA) for thermodynamic information on biologically related materials important to the space program for several reasons. Among these reasons are the necessity of inferring the maximum account of useful chemistry of incompletely accessible environments, for which only limited information is available, the possibility of the occurrence of organic compounds naturally synthesized under primitive conditions, and the possibility of theoretically recovering part of the pre-biological history of the earth.

This program is being carried out under the technical supervision of Dr. George Jacobs of NASA, and with the consultation of Dr. Harold Morowitz of the Yale University, Department of Molecular Biology and Biophysics, and Dr. C. W. Beckett of the Heat Division, Institute for Basic Standards (NBS). The contract (Contract No. R-138) was initiated 1 May 1964 and extended by Amendments 1, 2, and 3. This report covers a portion of work under Amendment 3. A significant change in the direction of the project occurred with the initiation of Amendment 3. The work is now directed toward the presentation of the material in the form of a Handbook of Thermodynamic Data of Interest in the Biological Sciences. In this effort the work at NBS is coordinated with a related task at the Texas A amd M Thermodynamic Properties Center under Dr. R. A. Wilhoit.

George T. Armstrong
Supervisory Chemist
Project Leader

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Report of Progress

George T. Armstrong

During this reporting interval substantial progress was made in the compilation of heats of combustion of organic substances relevant to the program. This work was done largely by Dr. E. S. Domalski, and is presented as a chapter of this progress report, beginning on page 2. The results presented here finish about 75 percent of the work on combustion reactions.

Plans for the preparation of the Handbook were discussed at a meeting between Dr. Armstrong and Dr. Wilhoit on December 12, 1968. The decision as to the publisher has been narrowed to two candidates. A decision will be made soon.

A visit was made to Dr. Wm. J. Evans of the Southern Regional Research Laboratory (U.S.D.A.) in New Orleans to discuss the forms of thermodynamic data in greatest need in the life sciences. This has also been the subject of correspondence with Dr. I. Wadsö of Lund University, and personal contacts with a number of other calorimetrists at the U.S. Calorimetry Conference (Midland, Michigan).

Selected Heats of Combustion and Heats of Formation of Organic Compounds of Biological Interest

Eugene S. Domalski

I. Introduction

As part of a continuing effort comprised of gathering and evaluating data on, and selecting best values for organic compounds of biological interest, we report here some selected heats of combustion and formation for the following classes of compounds: amino acids (taken from NBS Report 8641), peptides (taken from NBS Report 8641), certain organic compounds of biological interest (taken from NBS Report 8906), other amino acids and related compounds, amino acid anhydrides, glyceryl esters, lactones, heterocyclic nitrogen compounds, and heterocyclic oxygen compounds. The selected values are tabulated for each class of compounds in Section II of this report. The amino acids, peptides, and certain organic compounds of biological interest which were listed in earlier NBS reports have been included here for two reasons. First, selected values for L-cysteine, L-cystine and D-ribose needed revision in view of better or more recent measurements. Second, when a selected value was made on a compound which was measured in two or more independent investigations, no means was available in the earlier NBS reports to determine which data were preferred to others. In section III, called "Selection of the Combustion Data", we have indicated in brief form which data were used in making a given selection. When a selected value of a compound is derived from a single investigation, no comment is made.

In our last report (NBS Report 9883), selected values of the heats of combustion and formation of 73 organic compounds are listed. The latter were divided into four classes: alkaloids, monosaccharides, disaccharides, and porphyrins. In NBS Report 9374 selected values are given for benzene, naphthalene, anthracene and phenanthrene. These tables are not repeated in the present report. The total number of compounds for which selected values have been chosen in this report is 321. Adding to that total, the compounds in NBS Reports 9374 and 9883, we get 398 for a final total to date. Approximately 150 additional compounds are to be processed in this portion of the project.

II. Data on the Heats of Combustion and Formation of Various Classes of Organic Compounds

Amino Acids

Except for L-cysteine, L-cystine, and L-methionine, the data are the same as those which appeared earlier in NBS Report 8641, 1 February 1965.

Compound	State	ΔH_c° 298°K kcal mol^{-1}	ΔH_f° 298°K kcal mol^{-1}	Reference
L-alanine	c	-387.30	-133,96	[11,30,48,96,98]
DL-alanine	c	-386.71	-134.55	[32,50,85,87,98]
L-arginine	c	-893.85	-148.66	[50]
L-asparagine	c	-460.97	-188.50	[11,48,84,85,87,89]
L-asparagine hydrate	c	-458.26	-259.52	[30,48]
L-aspartic acid	c	-382.84	-232.47	[11,30,33,48, 85,87,109]
L-cysteine[(a)]	c	-540.5	-124.6	[6,17,47,110]
L-cystine[(a)]	c	-1016.3	-245.7	[6,17,30,47,110]
L-glutamic acid	c	-537.62	-240.05	[30,33,48,95,109]
L-glutamine	c	-614.0	-197.8	[95]
glycine	c	-232.67	-126.22	[11,30,33,50,84, 87,89,96,98]
hippuric acid	c	-1008.25	-145.63	[11,21,30,32,44, 45,46,81,84,85, 87,89,90,97,108]
L-hydroxyproline	c	-619.6	-158.1	[68]
DL- and L-isoleucine[(b)]	c	-856.5	-151.8	[68,96]
L-isoserine	c	-343.5	-177.8	[33,98]
D-leucine	c	-856.39	-151.97	[50]
L-leucine	c	-856.39	-151.97	[11,33,50,85,87,95]
DL-leucine	c	-855.62	-152.74	[50]
DL-lysine	c	-880.3	-162.2	[68]
L-methionine[(a)]	c	-809.5	-180.4	[96]

(footnotes (a) and (b) are explained on the following page.)

norleucine	c	-854.3	-154.1	[78]
DL-ornithine	c	-724.1	-156.0	[68]
DL- and L-phenylalanine[b]	c	-1110.3	-111.9	[18,33,96]
L-proline	c	-652.0	-125.7	[68]
sarcosine	c	-400.1	-121.2	[18,87]
serine	c		(c)	[51]
DL- and L-threonine[b]	c	-502.2	-181.4	[68,96]
L-tryptophan	c	-1344.6	-99.8	[96]
L-tyrosine	c	-1058.8	-163.4	[11,30,50,109]
DL- and L-valine[b]	c	-697.8	-148.2	[78,95,98]

(a) Final state of sulfuric acid was calculated to be $H_2SO_4 \cdot 115\ H_2O(l)$.

(b) It was impossible to assign different "best values" to DL and L forms because of the lack of precise data on both compounds.

(c) Authors of [51] estimate $\Delta H^\circ_{f_{298}} = -173.6$ kcal mole^{-1}.

Peptides

The data were taken from NBS Report 8641, 1 February 1965.

Compound	State	ΔH_c° 298°K kcal mol^{-1}	ΔH_f° 298°K kcal mol^{-1}	Reference
alanyl glycine	c	-626.19	-185.64	[46]
alanyl phenylalanine	c	-1505.0	-170.2	[67]
glycylglycine	c	-470.95	-178.51	[2,33,56]
glycyl phenylalanine	c	-1348.8	-163.9	[67]
glycyl valine	c	-936.6	-200.0	[67]
hippuryl glycine	c	-1245.92	-198.54	[46]
leucyl glycine	c	-1093.86	-205.07	[46,98]
seryl serine	c	-692.4	-281.8	[67]
valyl phenylalanine	c	-1816.3	-183.5	[67]
glycylalanyl phenylalanine	c	-1743.7	-222.0	[67]
leucyl glycyl glycine	c	-1329.9	-259.6	[33]

Certain Organic Compounds of Biological Interest

The data listed below are the same as those which appeared in NBS Report 8906, 1 July 1965, except for D-ribose.

Compound	State	ΔH_c° 298°K kcal mol^{-1}	ΔH_f° 298°K kcal mol^{-1}	Reference
adenine	c	-664.25	+23.21	[82]
creatine	c	-555.46	-128.16	[30,48,87]
creatine hydrate	c	-552.8	-199.1	[87]
creatinine	c	-558.54	-56.77	[30,48]
fumaric acid	c	-318.95	-193.89	[19,20,49,57,59,76,86,99,100]
α-D-glucose	c	-669.94	-304.26	[9,13,24,30,49,66,68 79,80,84,85,88,89]
α-D-glucose hydrate	c	-667.54	-374.97	[15,43,49,93]
β-D-glucose	c	-671.44	-302.76	[15,43,49,92,93]
guanine	c	-597.33	-43.72	[82,87]
hypoxanthine	c	-580.65	-26.24	[1,10,82]
maleic acid	c	-323.89	-188.94	[19,20,49,57,59,76,88,99]
nicotine	c	-1428.1	+9.4	[3,12]
8-oxypurine	c	-591.4	-15.4	[1,10]
D-ribose[(a)]	c	-557.9	-253.9	[55,111]
thymine	c	-563.3	-111.9	[33]
uric acid	c	-459.16	-147.73	[22,23,30,82,84,85,87,89]
xanthine	c	-516.39	-90.49	[3,12,82]
pyruvic acid	c	-278.5	-140.3	[16]

[(a)] Crystalline D-ribose is in the β-pyranose form [94].

Other Amino Acids and Related Compounds

Compound	State	ΔH_c° 298°K kcal mol^{-1}	ΔH_f° 298°K kcal mol^{-1}	Reference
glycine nitrate	c	-218.9	-174.1	[25]
diglycolamidic acid	c	-395.8	-219.5	[101,102]
glycylglycine-N-carboxylic acid	c	-470.5	-273.0	[33,98]
diglycylglycine	c	-709.2	-230.8	[98]
nitrilotriacetic acid	c	-559.2	-312.5	[101,102]
ethyl glycylglycinate	c	-803.7	-170.5	[2,33]
N-formyl-DL-leucine	c	-880.3	-222.1	[98]
triglycylglycine	c	-945.9	-284.7	[98]
β-carbethoxyglycylglycine ethyl ester	c	-1089.5	-303.5	[33]
α-carbethoxyglycylglycine ethyl ester	c	-1117.7	-275.3	[33]
ethylenediaminetetraacetic acid	c	-1066.5	-420.5	[26]
diethylenetriaminepentaacetic acid	c	-1570.5	-531.8	[26]
sarcosine polypeptide	c	-399.8	-53.1	[18]
N-phenyl glycine	c	-963.4	-96.2	[33]
α-phenyl glycine	c	-956.6	-103.2	[33]
phenaceturic acid	c	-1165.2	-151.0	[90,91]
DL-benzoylalanine	c	-1168.3	-147.9	[90,91]
p-toluylglycine	c	-1167.7	-148.5	[90,91]
m-toluylglycine	c	-1167.4	-148.8	[90,91]
anisoyl glycine	c	-1135.3	-180.9	[90,91]
benzoyl sarcosine	c	-1180.5	-135.7	[90,91]
o-toluyl glycine	c	-1167.9	-148.3	[90,91]
o-toluyl alanine	c	-1322.1	-156.5	[90,91]
p-toluyl alanine	c	-1319.6	-159.0	[90,91]
DL-phenylalanine-N-carboxylic acid dimethyl ester	c	-1456.7	-184.3	[18]

Compound	State	ΔH_c° 298°K kcal mol^{-1}	ΔH_f° 298°K kcal mol^{-1}	Reference
benzalhippuric acid	c	-1846.3	-102.6	[33]
benzalhippuric acid azlactone	c	-1850.0	-30.5	[33]
benzoylphenylalanine	c	-1887.6	-129.6	[33]
phenylalanine polypeptide (benzene soluble)	c	-1104.3	-49.6	[18]
phenylalanine polypeptide (benzene insoluble)	c	-1100.7	-53.2	[18]
L(+)-leucine methyl ester salt of (-)-1,1'-dinaphthyl-2,2'-dihydroxy carboxylic acid-(3,3')	c	-4358	-531	[28]
L(+)-leucine methyl ester salt of (+)-1,1'-dinaphthyl-2,2'-dihydroxy carboxylic acid-(3,3')	c	-4349	-540	[28]
ethyl β-anilino-β-phenyl propionate	c	-2165.1	-82.8	[27]

Amino Acid Anhydrides

Compound	State	$\Delta H^{\circ}_{c,298^{\circ}K}$ kcal mol^{-1}	$\Delta H^{\circ}_{f,298^{\circ}K}$ kcal mol^{-1}	Reference
glycine anhydride	c	-475.1	-106.0	[33,98]
sarcosine-N-carboxylic acid anhydride	c	-402.9	-144.1	[18]
seryl seryl anhydride	c	-696.4	-209.5	[112]
alanine anhydride	c	-787.6	-118.3	[2,33,98]
glycyl valyl anhydride	c	-947.7	-120.5	[112]
valyl alanyl anhydride	c	-1107.3	-123.3	[112]
valyl leucyl anhydride	c	-1567.6	-150.1	[112]
leucine anhydride	c	-1720.1	-160.0	[33]
phenylalanyl anhydride	c	-2238.5	-69.3	[112]
phenylalanine-N-carboxylic acid anhydride	c	-1115.6	-132.3	[18]
glycyl phenylalanyl anhydride	c	-1361.6	-82.9	[112]
glycyl tyrosyl anhydride	c	-1321.7	-122.8	[112]
alanyl phenylalanyl anhydride	c	-1517.5	-89.3	[112]
valyl phenylalanyl anhydride	c	-1837.2	-94.3	[112]

Glyceryl Esters

Compound	State	$\Delta H^{\circ}_{c,298^{\circ}K}$ kcal mol^{-1}	$\Delta H^{\circ}_{f,298^{\circ}K}$ kcal mol^{-1}	Reference
glyceryl monoacetate	l	-594.3	-217.5	[29]
glyceryl-1,3-diacetate	l	-800.0	-268.2	[29]
glyceryl triacetate	l	-1006.4	-318.3	[29]
glyceryl-1-benzoate	c	-1164.61	-185.80	[31]
glyceryl-2-benzoate	c	-1165.69	-184.72	[31]
glyceryl-1-caprate	c	-1845.71	-256.06	[31]
glyceryl-2-caprate	c	-1848.87	-261.90	[31]
tricyclobutyrin	l	-1847	-247	[34]
glyceryl tributyrate	l	-1943	-356	[34]
glyceryl-1-laurate	c	-2158.03	-277.47	[31]
glyceryl-2-laurate	c	-2160.02	-275.48	[31]
glyceryl-1-myristate	c	-2467.92	-292.31	[31,35]
glyceryl-2-myristate	c	-2470.34	-289.89	[31]
tricyclovalerin	l	-2311	-270	[34]
glyceryl-1-palmitate	c	-2778.67	-306.30	[31,35]
glyceryl-2-palmitate	c	-2781.72	-303.25	[31,35]
glyceryl-1-stearate	c	-3090.05	-319.75	[31]
glyceryl-2-stearate	c	-3093.89	-315.81	[31]
glyceryl tribenzoate	c	-2726	-214	[103]
glyceryl trilaurate	c	-5707	-489	[52,104,113]
glyceryl trimyristate	c	-6650	-520	[52,84,104,113]
glyceryl dierucate	c	-6979	-447	[104]
glyceryl dibrassidate	c	-10266	-596	[104]
glyceryl trierucate	c	-6954	-472	[104]
glyceryl tribrassidate	c	-10237	-625	[104]

Lactones

Compound	State	ΔH_c° 298°K kcal mol^{-1}	ΔH_f° 298°K kcal mol^{-1}	Reference
propiolactone	g	-351.17	-67.61	[53]
propiolactone	l	-339.93	-78.85	[53]
β-methylene-β-propiolactone (diketene)	l	-457.11	-55.72	[54]
levulinic lactone	l	-599.0	-76.2	[14]
D-arabonic acid-γ-lactone	c	-505.3	-238.2	[56]
D-mannonic-1,4-3,6-dilactone	c	-514.7	-254.6	[56]
L-ascorbic acid	c	-559.23	-278.34	[111]
D-glucaric acid-3,6-lactone	c	-494.0	-343.6	[56]
D-glucaric acid-1,4-lactone	c	-494.4	-343.2	[56]
saccharinic acid lactone	c	-656.3	-249.6	[105]
D-mannonic acid-γ-lactone	c	-609.7	-296.2	[56,58]
D-galactonic acid-γ-lactone	c	-607.6	-298.3	[56]
L-gulonic acid-γ-lactone	c	-614.4	-291.5	[58]
D-gluconic acid-δ-lactone	c	-605.6	-300.3	[56]
lactide	c	-653.4	-184.2	[4,5]
terebic acid	c	-777.7	-222.2	[36,37,38,39]
D-gluco-α-heptonic acid-γ-lactone	c	-726.0	-342.3	[58]
D-gluco-D-gulo-heptonic acid-γ-lactone	c	-712.7	-355.6	[56]
D-gluco-α,α-octonic acid-γ-lactone	c	-836.4	-394.2	[58]
dehydro-β-campholenolactone (inactive)	c	-1350.3	-136.7	[7]
dehydro-β-campholenolactone (dextrorotatory)	c	-1357.1	-129.9	[7]
methyl ethyl heptanone lactone (racemic)	c	-1303.5	-183.5	[41,42]
3(a)-hydroxy-trans-decalin-2(a)acetic acid lactone	c	-1610.36	-133.09	[40]
3(e)-hydroxy-trans-decalin-2(e)acetic acid lactone	c	-1606.19	-137.26	[40]

Heterocyclic Nitrogen Compounds

Compound	State	ΔH°_c 298°K kcal mol^{-1}	ΔH°_f 298°K kcal mol^{-1}	Reference
parabanic acid	c	-212.5	-138.0	[60,61]
hydantoin	c	-311.6	-107.2	[60]
uramil	c	-378.8	-168.2	[23]
barbituric acid	c	-360.6	152.2	[23,33]
dialuric acid	c	-198.4	-314.4	[23]
5-methyl hydantoin	c	-464.8	-116.3	[62]
allantoin	c	-409.64	-171.51	[30,60,82,114]
alloxan	c	-273.76	-239.08	[23,82,114]
5,5-dimethyl hydantoin	c	-617.1	-126.4	[62,116]
isouric acid	c	-459.0	-147.9	[23]
methyl allantoin	c	-566.6	-177.0	[60]
pseudouric acid	c	-453.5	-221.7	[23]
dimethyl parabanic acid	c	-538.2	-137.0	[60,115]
4-methyl uracil	c	-566.0	-109.2	[33]
4-methylhydrouracil	c	-618.0	-125.5	[33]
7-methyl purine	c	-820.6	+51.3	[1,10]
7-methylhypoxanthine	c	-759.4	-9.9	[1,10]
5-methyl-5-ethyl hydantoin	c	-770.9	-135.0	[62]
theobromine	c	-845.2	-86.4	[23,115]
alloxantin dihydrate	c	-583.7	-373.7	[23,114]
hydrulic acid	c	-658.2	-299.2	[23]
caffeine	c	-1017.8	-76.2	[23,87,115]
murexide	c	-736.0	-289.7	[23]
diethybarbituric acid (veronal)	c	-983.6	-178.7	[33]
4-phenyl uracil	c	-1132.1	-81.7	[33]
desoxyamalic acid	c	-1321.1	-285.7	[23]
amalic acid	c	-1239.8	-367.0	[23]

Compound	State	ΔH_c° 298°K kcal mol^{-1}	ΔH_f° 298°K kcal mol^{-1}	Reference
tetrazole	c	-219.0	+56.7	[63]
5-aminotetrazole	c	-246.2	+49.7	[63]
5-aminotetrazole nitrate	c	-224.1	-6.6	[63]
5-hydroxytetrazole	c	-163.9	+1.5	[64]
5-cyanotetrazole	c	-318.3	+96.1	[64]
3-amino-1,2,4-triazole	c	-343.1	+18.4	[64]
3-amino-1,2,4-triazole nitrate	c	-318.0	-40.9	[64]
1-methyl-5-aminotetrazole	c	-405.14	+46.25	[64]
2-methyl-5-aminotetrazole	c	-409.3	+50.4	[64]
5-methylaminotetrazole	c	-407.24	+48.35	[64]
5,5'-hydrazotetrazole	c	-459.8	+135.1	[63]
3-azido-s-triazole	c	-361.9	+105.5	[117]
4-amino-3-azido-s-triazole	c	-427.1	+136.5	[117]
3-azido-5-methyl-s-triazole	c	-512.6	+93.8	[117]
4-amino-3-azido-5-methyl-s-triazole	c	-568.6	+115.6	[117]
3-azido-5-ethyl-s-triazole	c	-668.5	+87.4	[117]
4-amino-3-azido-5-ethyl-s-triazole	c	-733.8	+118.5	[117]
1-(5-tetrazoyl)-4-guanyl-tetrazene monohydrate	c	-506.5	-45.2	[64]
1,2-di-(5-tetrazolyl)ethane	c	-687.3	+106.2	[64]
2,2-dimethyl-5,5'-azotetrazole	c	-761.5	+180.3	[64]
cis-1,1'-dimethyl-5,5'-azotetrazole	c	-769.7	+188.6	[64]
trans-1,1'-dimethyl-5,5'-azotetrazole	c	-770.5	+189.3	[64]
1-allyl-5-aminotetrazole	c	-678.7	+63.4	[64]
2-allyl-5-aminotetrazole	c	-682.9	+67.6	[64]
5-tetrazoylurethan	c	-562.7	-52.6	[63]

Compound	State	ΔH_c° 298°K kcal mol^{-1}	ΔH_f° 298°K kcal mol^{-1}	Reference
1,5-dimethylaminotetrazole	c	-532.2	+45.1	[63]
5-dimethylaminotetrazole	c	-564.9	+43.6	[64]
1,4-dimethyl-5-tetrazolone	c	-480.5	-6.6	[64]
3-amino-5-methyl-1,2,4-triazole nitrate	c	-466.7	-54.6	[64]
1,3-dimethyl-5-imino-tetrazole nitrate	c	-554.1	-1.3	[64]
acetamidoguanidine nitrate	c	-471.5	-118.1	[64]
ethylenimine	l	-380.86	+21.97	[65]
5-guanylaminotetrazole	c	-399.4	+40.5	[63]
5-methoxytetrazole	c	-341.3	+16.6	[64]
imidazole	c	-433.3	+14.5	[69]
pyrazole	c	-477.1	+28.3	[69]
5-acetamidotetrazole	c	-451.7	-1.2	[63]
melamine	c	-469.8	-17.3	[29,70,71]
pyridazine	g	-579.4	+66.6	[72]
pyridazine	l	-566.6	+53.8	[72]
pyrimidine	g	-559.9	+47.1	[72]
pyrimidine	l	-547.9	+35.1	[72]
pyrazine	g	-559.7	+46.8	[72]
pyrazine	c	-546.2	+33.3	[72]
pyrrole	g	-572.87	-25.88	[73]
pyrrole	l	-562.07	+15.08	[73]
piperazine hexahydrate	c	-690.9	-436.8	[74.75]
pyrrolidine	g	-683.62	-0.89	[83]
pyrrolidine	l	-673.75	-9.87	[77.83]
α-pyrrolidone	c	-547.0	-68.3	[106]
piperazine	c	-706.9	-10.9	[107]
pyridine	g	-674.65	+33.61	[119,122]
pyridine	l	-665.00	+23.96	[118-124]
1,2,5,6-tetrahydropyridine	l	-785.7	+8.0	[107]

Compound	State	ΔH_c° 298°K kcal mol^{-1}	ΔH_f° 298°K kcal mol^{-1}	Reference
pyrrolaldehyde	c	-616.3	-24.8	[125]
piperidine	l	-824.94	-21.05	[107,120,121]
α-piperidone	c	-704.4	-73.3	[106]
N-methylpyrrolidone	l	-715.03	-62.64	[126]
pyrrolaldoxime	c	-678.9	+3.7	[125]
2,6-diaminopyridine	c	-707.9	-1.5	[130,131]
dimethyldiketopiperazine	c	-777.9	-128.0	[116]
benzotriazole	c	-794.8	+59.7	[132]
N-methyl piperidone	l	-870.04	-70.00	[126]
e-caprolactam	c	-861.4	-78.6	[106]
triethylenediamine	c	-970.8	-3.4	[127]
hexamethylenetetramine	c	-1002.9	+28.7	[133-137]
hexamethylenetetramine dinitrate	c	-953.9	-88.6	[135,136,137]
3-cyanopyridine	c	-747.2	+46.2	[70,71]
2-methylpyridine	g	-827.46	+24.05	[119,139]
2-methylpyridine	l	-817.24	+13.83	[118,119,138,139]
3-methylpyridine	g	-829.71	+26.30	[119,140]
3-methylpyridine	l	-818.98	+15.57	[118,119,138,140]
4-methylpyridine	g	-827.85	+24.44	[119]
4-methylpyridine	l	-816.99	+13.58	[118,119,138]
picolinic acid	c	-651.4	-83.7	[128]
2-ethyl pyridine	l	-964.6	-1.2	[141]
2,3-dimethylpyridine	l	-970.40	+4.62	[129]
2,4-dimethylpyridine	l	-969.63	+3.85	[129]
2,5-dimethylpyridine	l	-970.23	+4.45	[119,129]
2,6-dimethylpyridine	l	-968.80	+3.02	[118,119,129]
3,4-dimethylpyridine	l	-970.14	+4.36	[129]
3,5-dimethylpyridine	l	-971.14	+5.36	[129]
1-phenyltetrazole	c	-949.8	+86.5	[63]

Compound	State	ΔH_c° 298°K kcal mol^{-1}	ΔH_f° 298°K kcal mol^{-1}	Reference
5-phenyltetrazole	c	-933.3	+70.0	[63]
2-vinyl pyridine	l	-934.7	+37.2	[141]
1-methyl-5-phenyl tetrazole	c	-1095.6	+69.9	[64]
1-phenyl-5-methyl tetrazole	c	-1095.6	+69.9	[63,64]
2-phenyl-5-methyl tetrazole	c	-1091.3	+65.7	[63]
1-phenyl-5-aminotetrazole	c	-971.8	-74.3	[64]
5-phenylaminotetrazole	c	-970.4	-72.9	[64]
1-phenyl-5-hydroxytetrazole	c	-890.0	+26.7	[63]
1-allyl-5-allylaminotetrazole	c	-1117.8	+83.7	[64]
5-diallylaminotetrazole	c	-1118.0	+83.9	[64]
N-methylcaprolactam	l	-1029.1	-73.3	[126]
7-methylcaprolactam	c	-1015.9	-86.5	[106]
5-methylcaprolactam	c	-1015.5	-86.9	[106]
zeta-enantolactam	c	-1019.2	-83.2	[106]
3-azido-5-phenyl-s-triazole	c	-1084.5	+127.1	[117]
4-amino-3-azido-5-phenyl-s-triazole	c	-1151.0	+159.5	[117]
indole	c	-1021.3	+29.8	[3,12,142]
α-methylindole	c	-1168.4	+14.5	[3,12]
isatin	c	-860.5	-62.7	[125,143]
dioxindole	c	-914.6	-76.9	[143]
oxindole	c	-950.3	-41.2	[3,12]
dipyrrylketone	c	-1115.0	-4.7	[142]
dipyrrylmethane	c	-1219.4	+31.4	[142]
quinoline	c	-1122.9	+37.3	[120,146]
isoquinoline	c	-1123.5	+37.9	[120,144]
phyllopyrrole	c	-1338.4	-20.4	[120]
8-hydroxyquinoline	c	-1065.7	-19.9	[145,153,154]

Compound	State	ΔH_c° 298°K kcal mol^{-1}	ΔH_f° 298°K kcal mol^{-1}	Reference
skatole	c	-1170.2	+16.3	[3,12]
α-phenylpyrrole	c	-1282.4	+34.5	[142]
quinaldine	c	-1287.2	+39.3	[120,146]
carbazole	c	-1466.3	+30.3	[3,12,147]
phenazine	c	-1458.3	+56.4	[148,149]
acridine	c	-1574.9	+44.8	[148,149]
isatide	c	-1775.6	-139.1	[143]
indigotin	c	-1814.0	-32.4	[143]
amygdalin	c	-2348	-455	[150,151]
lophine	c	-2587	+65	[120]
amarine	c	-2653	+63	[120,152]
amarine hemihydrate	c	-2653	+29	[120,152]
anisine	c	-2653	+63	[120,152]

Heterocyclic Oxygen Compounds

Compound	State	ΔH_c° 298 °K kcal mol^{-1}	ΔH_f° 298 °K kcal mol^{-1}	Reference
ethylene carbonate	c	-279.9	-138.9	[155]
trimethylene oxide	g	-467.85	-12.58	[156]
furan	g	-504.60	-8.23	[157,172]
furan	l	-497.99	-14.84	[157,158]
tetrahydrofuran	g	-605.44	-44.03	[156]
tetrahydrofuran	l	-598.4	-51.1	[80,159]
glycol acetal	l	-558.4	-91.1	[160]
1,3-dioxane	l	-559.48	-89.99	[161,162,163]
1,4-dioxane	l	-564.99	-84.47	[161,164,165]
pyromucic acid	c	-487.8	-119.1	[85,158,166,167,168]
furfuryl alcohol	l	-609.2	-66.0	[158,166,167]
tetrahydrofurfuryl alcohol	l	-707.7	-104.1	[158]
dihydropyran	l	-706.0	-37.5	[159]
tetrahydropyran	g	-758.44	-53.50	[156]
tetrahydropyran	l	-750.7	-61.1	[80,159,161,169]
furfural	l	-559.1	-47.8	[158,168,170,171]
erythritol diformal	c	-744.1	-161.8	[160]
erythritol diacetal	c	-1048.5	-182.1	[160]
mannitol triformal	c	-1082.8	-241.9	[160]
mannitol triacetal	c	-1537.2	-274.6	[160]

III. Selection of the Combustion Data

Amino Acids and Peptides (NBS Report 8641)

L-alanine - The data of Huffman, Ellis and Fox [48] were chosen in preference to earlier work. The combustion data of Tsuzuki, Harper and Hunt [96] were in disagreement with our selection by more than 10 kcal mol^{-1}.

DL-alanine - The data of Huffman, Fox and Ellis [50] were chosen in preference to the earlier work.

L-asparagine - The data of Huffman, Ellis and Fox [48] were chosen in preference to earlier work.

L-asparagine monohydrate - The data of Huffman, Ellis, and Fox [48] were chosen in preference to the data of Emery and Benedict [30].

L-aspartic acid - The data of Huffman, Ellis and Fox [48] were chosen in preference to those of other workers.

L-cysteine - The combustion data of Sunner [110] were chosen in preference to the earlier work.

L-cystine - The combustion data of Sunner [110] were chosen in preference to the earlier work.

L-glutamic acid - The data of Huffman, Ellis and Fox [48] were chosen in preference to other work.

glycine - The data of Huffman, Fox and Ellis [50] were chosen in preference to the other work.

hippuric acid - The data of Hubbard, Frow and Waddington [44], Wagner [97], Fairbrother, Skinner and Evans [32], Cole and Gilbert [108], and Huffman [45,46] were averaged in making the selection. The data of Coates and Sutton [21] and Springhall, White and Cass [81] were not used.

DL- and L-isoleucine - The data of Ponomarev and Migarskaya [68] on DL-isoleucine were used for the selected value of both DL- and L-isoleucine. A value for $\Delta H^{\circ}_{f\ 298}$[L-isoleucine (c)] of -152.9 kcal mol^{-1} was calculated from the data of Tsuzuki, Harper and Hunt [96], but was not used because of the poor agreement found between heats of formation calculated for other amino acids by these authors and the values calculated by other investigators.

L-isoserine - The work of Wrede [98] was used in making the selection.

L-leucine - The data of Huffman, Fox, and Ellis [50] were chosen in preference to other work.

DL- and L-phenylalanine - The data of Tsuzuki, Harper, and Hunt [96], Breitenbach, Derkosch, and Wessely [18], and Fischer, and Wrede [33] were averaged in making the selection. It was impossible to assign different values to the DL- and L-forms because of the lack of accuracy in the data.

sarcosine - The data of Breitenbach, Derkosch, and Wessely [18], and Stohmann, and Langbein [87] were averaged to make the selection.

DL- and L-threonine - The data of Ponomarev and Migarskaya [68] were used for the selected value of both DL- and L-threonine. A value for $\Delta H^{\circ}_{f\ 298}$[L-threonine (c)] of -193.15 kcal mol^{-1} was calculated from the data of Tsuzuki, Harper and Hunt [96], but was not used because of the poor agreement found between heats of formation calculated for other amino acids by these authors and the values calculated by other investigators.

L-tyrosine - The data of Huffman, Fox, and Ellis [50] were used in preference to other work.

DL- and L-valine - The data of Skuratov [78] and Tsuzuki and Hunt [95] both, on L-valine were averaged for the selected value for DL- and L-valine. The data of Wrede [98] on DL-valine is regarded as not accurate enough to assign a different value to these two forms.

glycylglycine - The data of Huffman [46] were used in making the selection in preference to the earlier data.

leucylglycine - The data of Huffman [46] were used in making the selection in preference to the data of Wrede [98].

Certain Organic Compounds of Biological Interest (NBS Report 8906).

creatine - The combustion data of Huffman, Ellis, and Fox [48] were chosen in preference to the earlier work.

creatinine - The data of Huffman, Ellis and Fox [48] were chosen in preference to the data of Emery and Bendict [30].

fumaric acid - The data of Wilhoit and Shiao [99], Schwabe and Wagner [76] and Huffman and Fox [49] were average to make the selection. The data on fumaric acid prior to 1900 were not used.

α-D-glucose - The data of Skuratov, Strepikheev and Kozina [80] and Huffman and Fox [49] were averaged to make the selection. The data on α-D-glucose prior to 1900 were not given consideration. The data of Emery and Bendict [30] differed by about 2 kcal mol^{-1} and that of Ponomarev and Alekseeva [66] differed by about 1 kcal mol^{-1}, from the selected value.

α-D-glucose hydrate and β-D-glucose - The selected heats of combustion and heats of formation of β-D-glucose and α-D-glucose hydrate were obtained from the heat of solution data of Hendricks, et al. [15,43], Taylor and Rowlinson [93] and Sturtevant [92] on α-D-glucose, β-D-glucose and α-D-glucose hydrate in conjunction with the combustion data of Huffman and Fox [49] on α-D-glucose.

guanine - The data of Stiehler and Huffman [82] were chosen in preference to the data of Stohmann and Langbein [87].

hypoxanthine - The data of Stiehler and Huffman [82] were chosen in preference to the data of Berthelot [1,10].

maleic acid - The data of Wilhoit and Shiao [99] were chosen in preference to the earlier data.

D-ribose - The combustion data of Desai and Wilhoit [111] were chosen in preference to the data of Stroh and Fincke [55].

uric acid - The data of Stiehler and Huffman [82] were chosen in preference to the earlier work.

xanthine - The data of Stiehler and Huffman [82] were chosen in preference to the data of Berthelot and Andre [3,12].

Other Amino Acids and Related Compounds.

glycylglycine-N-carboxylic acid - The combustion data of Fischer, and Wrede [33] and Wrede [98] were averaged to make the selection.

ethyl glycylglycinate - The combustion data of Fischer, and Wrede [33], and Landrieu [2] were averaged to give the selected value.

α-phenylglycine - The combustion data of Fischer and Wrede [33], and Landrieu [2] were averaged to give the selected value.

Amino Acid Anhydrides

glycine anhydride - The combustion data of Fischer and Wrede [33], Landrieu [2], and Wrede [98] were averaged to give the selected value.

L-alanine anhydride - The combustion data of Fischer and Wrede [33], Landrieu [2], and Wrede [98] were averaged to give the selected value.

Glyceryl Esters

glyceryl-1-myristate - The combustion data of Silbert, Daubert and Mason [31] were chosen in preference to the data of Clarke and Stegeman [35].

glyceryl-1-palmitate - The combustion data of Silbert, Daubert and Mason [31] were chosen in preference to the data of Clarke and Stegeman [35].

glyceryl-2-palmitate - The combustion data of Silbert, Daubert and Mason [31] were chosen in preference to the data of Clarke and Stegeman [35].

glyceryl trilaurate - The combustion data of Louguinine [52,113] and Stohmann and Langbein [104] were averaged to give the selected value.

glyceryl trimyristate - The combustion data of Stohmann and Langbein [104] were used for the selected value in preference to the data of Louguinine [52,113] and Stohmann [84].

Lactones

D-mannonic acid-γ-lactone - The combustion data of Stroh and Kilchenmeister [56] was used for the selection. The early combustion data of Fogh [58] on D- and L-mannonic acid-γ-lactone was not used because of such poor agreement with the value of Stroh and Kilchenmeister [56].

terebic acid - The early combustion data of Osipov [36,37] was not used. The selection was made from the later publications [38,39].

Heterocyclic Nitrogen Compounds

barbituric acid - The combustion data of Fischer and Wrede [33] were selected in preference to the work of Matignon [23].

allantoin - The combustion data of Stiehler and Huffman [82] were chosen in preference to the earlier work for the selected value.

alloxan - The combustion data of Stiehler and Huffman [82] were chosen in preference to the earlier work of Matignon [23,114].

5,5-dimethylhydantoin - The combustion data of Tavernier and Lamouroux [62] and McEwan [116] were averaged to make the selection.

caffeine - The combustion data of Matignon [23,115] and Stohmann and Langbein [87] were averaged to make the selection.

melamine - The combustion data of Salley and Gray [70,71] and Tavernier and Lamouroux [29] were averaged to make the selection.

pyrrole - The combustion data of Scott, et al. [73] was used for the selection in preference to the earlier work of Berthelot and Andre [3].

pyrrolidine - The combustion data of McCullough, et al. [83] was chosen for the selection. The value obtained by Hildenbrand, et al. [77] for the enthalpy of combustion of pyrrolidine is in excellent agreement with the selection.

pyridine - The combustion data of Cox, Challoner, and Meetham [119], and Hubbard, Frow, and Waddington [122] were averaged to make the selection. The early work of Delepine [120,121] was in good agreement with the selection by about 0.1 kcal mol^{-1}; this is perhaps fortuitous. The remaining combustion data [118,123,124] varied between 7 and 14 kcal mol^{-1} from the selected value. The heat of vaporization of pyridine was, similarly, an average value made by summing the data of Cox, et al. [119], and Hubbard, et al. [122]; the heat of vaporization of pyridine was taken to be 9.65 kcal mol^{-1}.

piperidine - The combustion data of Bedford, Beezer, and Mortimer [107] were chosen for the selected value. The data of McCullough and coworkers, ΔH_c°[piperidine (1)] at 25°C = -825.29 ± 0.11 kcal mol^{-1}, cited in reference [107] are in good agreement with the selected value. We have not used the data of McCullough and coworkers because their work has not yet appeared as a formal publication. The data of Delepine [120,121] were not used.

hexamethylenetetramine - The combustion data of Delepine, and Badoche [135] were used for the selected value in preference to their earlier work.

hexamethylenetetramine dinitrate - The combustion data of Delepine, and Badoche [135] were used in preference to the earlier work of Delepine [136,137].

2-methylpyridine - The combustion data of Scott, et al. [139] and Cox, Challoner, and Meetham [119] were averaged in making the selection. Similar treatment was given to the data on the heat of vaporization of the above authors. The data of Constam, and White [118], and Roth and Miller [138] were not used.

3-methylpyridine - The combustion data of Scott, et al. [140], and Cox, Challoner, and Meetham [119] were used in making the selection. Similar treatment was given to the data on the heat of vaporization of the above authors. The data of Constam, and White [118], and Roth and Miller [138] were not used.

4-methylpyridine - The combustion data of Cox, Challoner, and Meetham [119] were using in making the selection in preference to the earlier data of Constam and White [118], and Roth and Müller [138].

2,5-dimethylpyridine - The combustion data of Cox and Gundry [129] were used in preference to the earlier work of Cox, Challoner, and Meetham [119].

2,6-dimethylpyridine - The combustion data of Cox and Gundry [129] were used in preference to the earlier work of Cox, Challoner, and Meetham [119] and Constam and White [118].

1-phenyl-5-methyltetrazole - The combustion data of McEwan and Riggs [63] and Williams, McEwan and Henry [64] were averaged to make the selection.

indole - The combustion data of Stern and Klebs [142], and Berthelot and Andre [3,12] were averaged to make the selection.

isatin - The combustion data of Stern and Klebs [125] were used in preference to the data of d'Aladern [143].

8-hydroxyquinoline - The combustion data of Sullivan and Hunt [154] and Wood and Jones [145] were averaged to obtain the selected value.

carbazole - The combustion data of Tavernier and Lamouroux [147] were used in making the selection in preference to the data of Berthelot and Andre [3,12].

Heterocyclic Oxygen Compounds

furan - The combustion data of Guthrie, et al. [157] were chosen in preference to the data of Landrieu, et al. [158]. The unpublished data of Pilcher [172] on the heats of combustion and formation of furan (g) at 25°C, ΔH_c° = -504.45 ± 0.15, and -8.39 ± 0.16 kcal mol^{-1}, are in excellent agreement with the work of Guthrie, et al. [157].

tetrahydrofuran (1) - The combustion data of Skuratov, Strepikheev and Kozina [80], and Cass, Fletcher, Mortimer, Springall, and White [159] were averaged in making the selection.

1,3-dioxane and 1,4-dioxane - The combustion data of Snelson and Skinner [161] were chosen in preference to other data.

pyromucic acid - The combustion data of Parks, Mosley, and Peterson [166] were chosen in preference to other data.

furfuryl alcohol - The combustion data of Parks, Mosley and Peterson [166] were chosen in preference to other data.

tetrahydropyran (1) - The combustion data of Skuratov and Kozina [169], and Snelson and Skinner [161] were averaged to make the selection.

furfural - Values of the heat of combustion ranged over three kilocalories per mole. No one piece of work seemed more accurate than another. The selection was made by averaging the data of Landrieu, Baylocq and Johnson [158], Berthelot and Rivals [168], Chung-Cheng [170] and Miller [171].

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